

1,2,4,5-tetrachloro-3-methoxy-6-nitrobenzene

Inchi:	InChI=1S/C7H3Cl4NO3/c1-15-7-4(10)2(8)6(12(13)14)3(9)5(7)11/h1H3
InchiKey:	BGPPUXMKKQMWLV-UHFFFAOYSA-N
Formula:	C7H3Cl4NO3
SMILES:	COc1c(Cl)c(Cl)c([N+](=O)[O-])c(Cl)c1Cl
Mol. weight [g/mol]:	290.92
CAS:	2438-88-2

Physical Properties

Property code	Value	Unit	Source
hfus	35.32	kJ/mol	Joback Method
log10ws	-5.38		Cheméo Relay (1.0)
logp	4.217		Crippen Method
mcvol	157.980	ml/mol	McGowan Method
tb	581.77		Cheméo Relay (1.0)
tf	376.15		Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	1.16670e+02
Coeff. B	3.55780e-01
Coeff. C	-1.02000e-04
Coeff. D	-2.59000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):
Joback Method:

https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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